

## Temperature Measurement in a Microtubular Flow Reactor

Kimberly N. Urness,<sup>1,2,\*</sup> AnGayle K. Vasiliou,<sup>3</sup> David L. Osborn,<sup>4</sup> Musahid Ahmed,<sup>5</sup> Amir Golan,<sup>5</sup> John W. Daily,<sup>2</sup> John F. Stanton,<sup>6</sup> John R. Barker,<sup>7</sup> and G. Barney Ellison<sup>1</sup>

<sup>1</sup> Department of Chemistry & Biochemistry, University of Colorado, Boulder, CO, USA

<sup>2</sup> Department of Mechanical Engineering, University of Colorado, Boulder, CO, USA

<sup>3</sup> Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA

<sup>4</sup> Combustion Research Facility, Sandia National Laboratory, Livermore, CA, USA

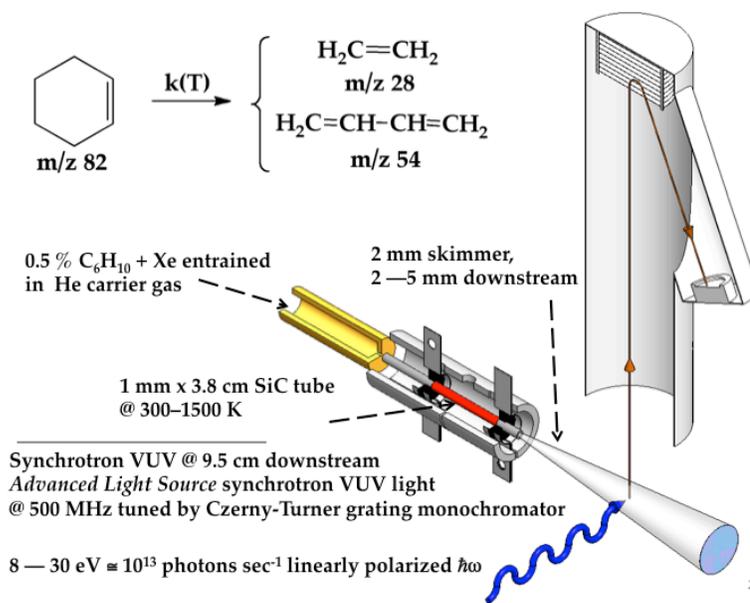
<sup>5</sup> Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

<sup>6</sup> Department of Chemistry, University of Texas, Austin, TX, USA

<sup>7</sup> Department of Atmospheric, Oceanic & Space Sciences, University of Michigan, Ann Arbor, MI, USA

\* Corresponding author: Kimberly.Urness@colorado.edu

We are developing a microtubular reactor to pyrolyze biomass samples (sugars and lignins). To characterize the thermodynamic conditions in the microtubular flow tube, we have pyrolyzed cyclohexene as a chemical thermometer.[1] The reaction kinetics of the retro-Diels-Alder fragmentation of cyclohexene to ethylene and 1,3-butadiene is well studied.[2] Cyclohexene is decomposed in a heated silicon carbide (SiC) reactor under continuous flow conditions over a range of reactor wall temperatures from 300 to 1500 K; the residence time,  $t$ , in the flow reactor has been estimated to be 50–200  $\mu\text{sec}$ . A dilute gas mixture of 0.5% cyclohexene and xenon (as an internal standard) in helium emerges from the reactor as a skimmed molecular beam at a pressure of approximately 1  $\mu\text{Torr}$ , where all reactions cease. Photoionization mass spectroscopy is used to detect cyclohexene, ethylene, and 1,3-butadiene relative to the internal standard, Xe. The cyclohexene, being in a constant temperature reactor for a known residence time, decomposes and the rate constant can be deduced. From the temperature and pressure dependence of the rate constant, the effective, chemical temperature of the microtubular reactor can be deduced. There are two problems with this simple analysis. First, the rate constant must be known with confidence. Second, the pressure and, perhaps, temperature, are not constant in the reactor. Experimental results and the analysis will be presented.



Photoionization mass spectroscopy is used to detect cyclohexene, ethylene, and 1,3-butadiene relative to the internal standard, Xe. The cyclohexene, being in a constant temperature reactor for a known residence time, decomposes and the rate constant can be deduced. From the temperature and pressure dependence of the rate constant, the effective, chemical temperature of the microtubular reactor can be deduced. There are two problems with this simple analysis. First, the rate constant must be known with confidence. Second, the pressure and, perhaps, temperature, are not constant in the reactor. Experimental results and the analysis will be presented.

### References

- (1) Tranter, R.S., Sivaramakrishnan, R., Srinivasan, N., Brezinsky, K. *Int. J. Chem. Kinet.* **2001**, *33*, 722-731.
- (2) Kiefer, J.H., Shah, J.N. *J. Phys. Chem.* **1987**, *91*, 3024-3030.